Computational Modeling and Simulation

Fact Sheet

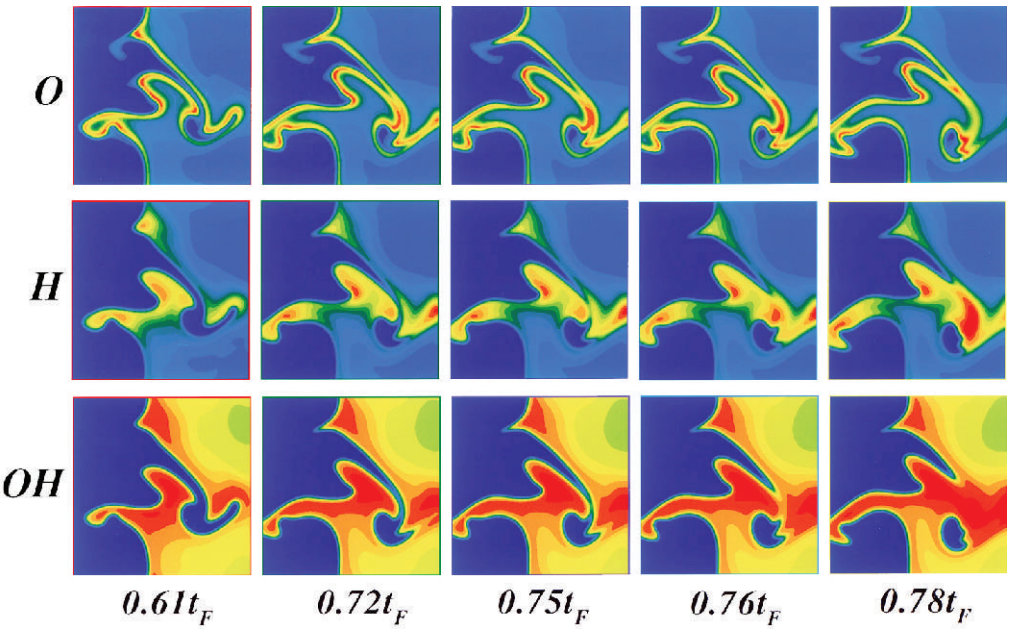
Understanding complex problems such as combustion events is greatly aided by computational modeling and simulation. A model is a simplified way of describing and predicting scientific results. For a complete simulation of a typical combustion device to be feasible, even on the largest of computers, the inclusion of simplifying models is required.

Working closely with experimentalists, theorists at the Combustion Research Facility are assessing how the combination of flow and chemistry in burning fuels affects the performance of combustion devices. The goal is to reliably predict factors that can guide design, operation, and fuel selection.

Direct Numerical Simulation

Direct numerical simulation (DNS) is a predictive approach that is appealing because of its accuracy and simplicity. DNS involves calculating the fully-resolved evolution of turbulent reactions, but is usually limited by computer capabilities to the details of flow and chemistry in a small zone. From the results of these simulations, one can obtain physical insight into the detailed aspects of combustion and validate models of these processes. These sub-models can then be combined into a larger simulation. The goal of the larger, or device-scale, simulation is to be realistic over the time frame and volume needed to understand device performance.

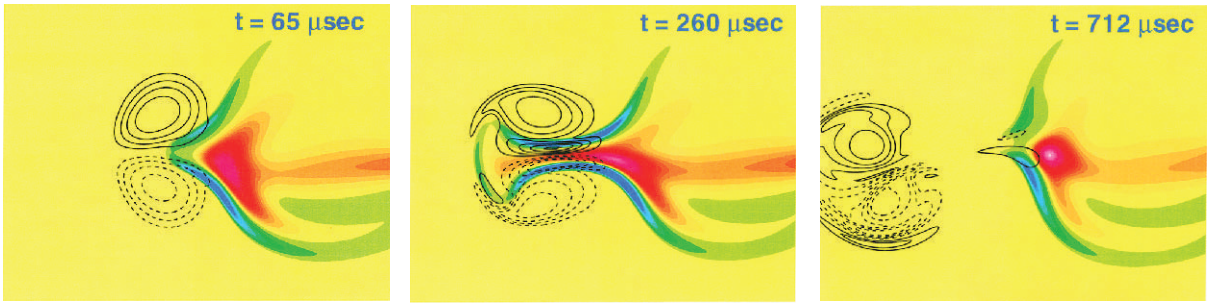
The level of detail is immense. Tackling these problems, large computers are akin to molecular microscopes. For a simple fuel like methane, at least 100 elementary reactions might be considered, along with factors such as chemical concentrations, flow momentum, and temperature. A simulation gives form to the phenomena by defining a mesh whose contours follow the



The time evolution of oxygen-atom, and hydroxyl-radical concentrations is shown for a 2D simulation of a lean, premixed methane-air flame. Concentration increases from blue to red. The unburnt gases were on the left initially, and the interaction of the flame front with the moving gases forms the burning pocket seen in the lower right corner.

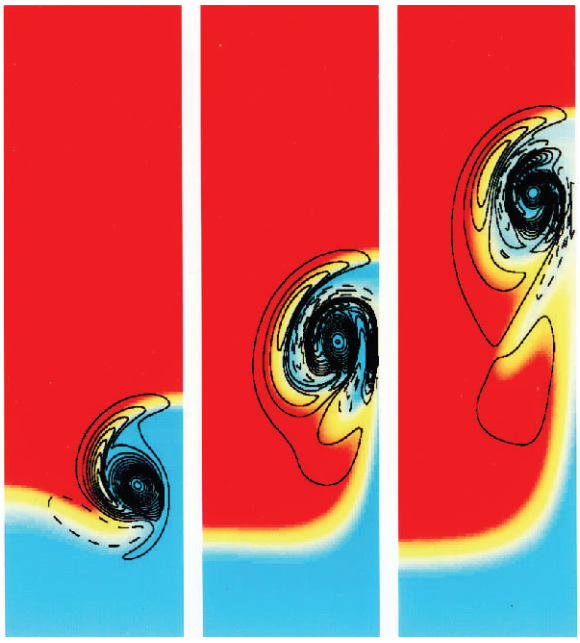
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories



Time sequence of a hydrogen-air triple flame interacting with a pair of counter-rotating vortices. The color contours show the reaction rate of the H-atom normalized by the maximum value for the unstrained, freely-propagating flame, while the line contours indicate the vorticity field. The H-atom reaction rate contours reveal the three branches of the flame structure.

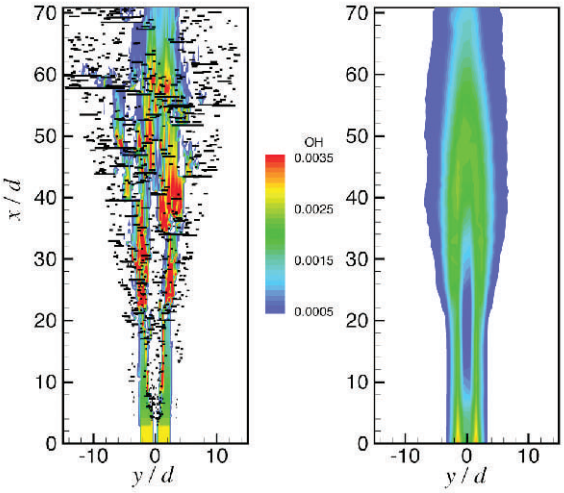
dimensions examined, much like a net would appear if it were placed on top of a relief map. Using a three-dimensional basic mesh of about one billion points one would need to solve for about 40 or 50 variables at each point to represent a fraction of the phenomena in question. An example might be the simulation of how two or three eddies of fuel and air will swirl together and burn within two milliseconds. That problem would require a supercomputer with a terascale capacity and gigabytes of memory and many days to compute.



A 1 ms time sequence of a premixed methane-air flame interaction with a counter-rotating vortex-pair, using detailed C1C2 chemical kinetics. The color map and contour lines indicate temperature and vorticity respectively. The interaction results in large unsteady strain-rate and curvature disturbances to the flame, with consequent effects on reaction rates and internal flame structure.

Statistical Modeling

A statistical approach to modeling turbulence—fluid motions that enhance mixing—at Sandia also shows promise. The statistical method is novel because it focuses on one dimension, and yet reliably predicts diverse processes in a physically sound manner. The calculations are highly parallel, so they can be affordably run on banks of networked computers.



Time evolution of a one-dimensional statistical simulation, rendered as downstream evolution (x) of the transverse (y) structure of a piloted methane-air jet diffusion flame. Axes scaled by inner-flow diameter d. Horizontal segments mark stirring events (turbulent 'eddies'). OH mass fraction field is shown for a single simulation (left) and an average over many simulations (right).

Contact:

Larry Rahn, Manager
Computational Modeling and Simulation
(925) 294-2091
e-mail: rahn@sandia.gov

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories